

Gas Chromatograph Mass Spectrometer

# GCMS-TQ8040 NX

*UFMS*  
ULTRA FAST MASS SPECTROMETRY



Smart Performance That Boosts Routine Analytical Work

# GCMS-TQ8040 NX

**Smart Performance**—Enabling highly sensitive simultaneous analysis of multiple components

**Smart Productivity**—Achieving superior productivity through dedication to efficiency

**Smart Operation**—Supporting easy creation of methods and data analysis

The fusion of these three Smart features makes this universal triple quadrupole GC-MS applicable in any field, where it is sure to deliver the utmost in performance.





POWER  
READY  
RELEASE

SHIMADZU

SHIMADZU

GCMS-TQ8040 NX  
MULTI-CAPABILITY GC/MS SYSTEM

Nexis GC-2030 GAS CHROMATOGRAPH

Start Stop Home

**RUN** LINE 1

200.0°C	SPL	FID	200.0°C
50.0 µL			X10 <sup>-1</sup>
150.0 cm			100 µm
80.0°C			FID1

Injection 1.000 µL 6.4

Retention Time 6.35

Peak 1

Chromatogram

Maintenance Temp Controller Flow Monitor

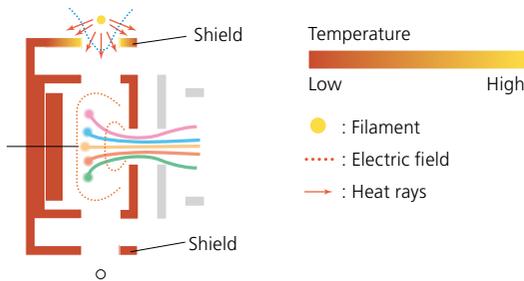
Power button

# Smart Performance

Equipped with an ion source that features high sensitivity and long-term stability, and a high-efficiency collision cell, the system can provide sensitive, stable analyses over a long period of time. Also, since it incorporates the Nexis™ GC-2030, high-precision control over flowrate and temperature is assured, enabling the acquisition of highly reliable data.

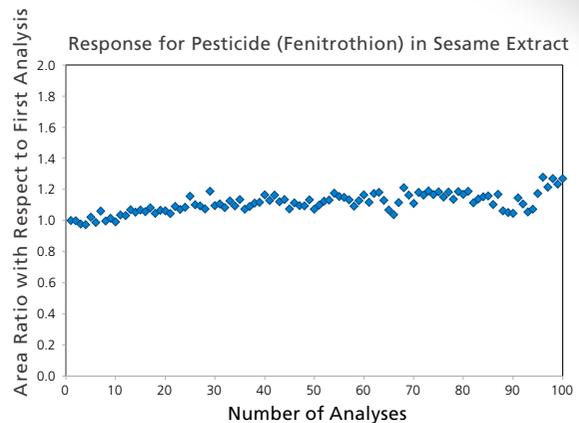
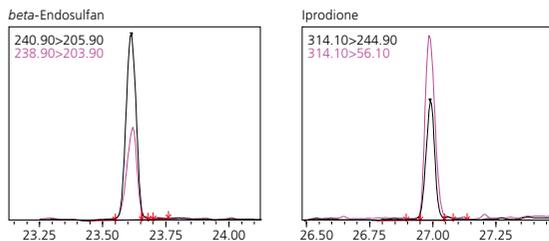
## ■ Highly Sensitive and Stable Ion Source

The effect of the filament's electric potential on the ion source is reduced by placing more distance between the filament and ion source box. In addition, a shield blocks out radiant heat generated from the filament to ensure the ion source box temperature remains uniform. Since this prevents any active spots within the ion source, it provides higher sensitivity for analysis. (Patent: US7939810)



## ■ High-Performance Quadrupole Mass Filter

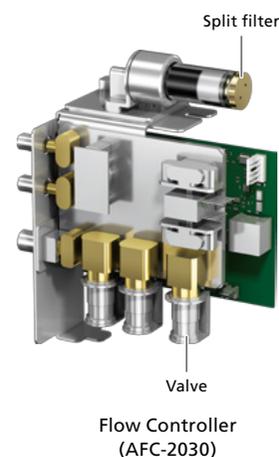
The high-accuracy mass filter with pre-rods and patented electric field control technology achieves high-accuracy mass separation performance. Also, the pre-rods minimize quadrupole contamination and eliminate the need for quadrupole maintenance.



## ■ New Flow Controller Achieves Exceptional Reproducibility

A new flow controller (AFC) with a CPU uses various control methods to control carrier gas flow to a constant flow speed, flowrate, or pressure. It can also accurately trace the analytical conditions already being used.

The split line filter can be replaced without any tools. Internal contamination can be confirmed visually, ensuring filters are replaced at the proper time.



Flow Controller  
(AFC-2030)

## ■ One Touch Inlet Maintenance

The injection port can be opened or closed without tools by simply sliding the ClickTek™ lever. Replace the insert, slide the lever and feel the click for a leak-free install every time.

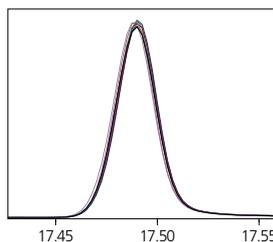


ClickTek Nut

## ■ Advanced GC Oven

The improved temperature control function enables more precise temperature control of the GC oven, which improves the precision of retention time reproducibility.

In addition, three oven cooling rate levels can be specified to minimize damage to column liquid phases and maximize the service life.



Mass Chromatogram of Benzo[a]pyrene  
(Overlaid Plotting of Measurements Repeated Eight Times)

	Area value %RSD	Retention time %RSD
Acenaphthylene	0.969	0.005
Fluorene	0.918	0.007
Phenanthrene	1.075	0.006
Anthracene	1.141	0.007
Pyrene	1.263	0.004
Benzo[a]anthracene	1.405	0.005
Chrysene	1.283	0.005
Benzo[b]fluoranthene	1.940	0.003
Benzo[k]fluoranthene	1.268	0.003
Benzo[a]pyrene	0.781	0.005
Indeno[1,2,3-cd]pyrene	0.744	0.004
Dibenz[a,h]anthracene	0.836	0.004
Benzo[ghi]perylene	0.767	0.004

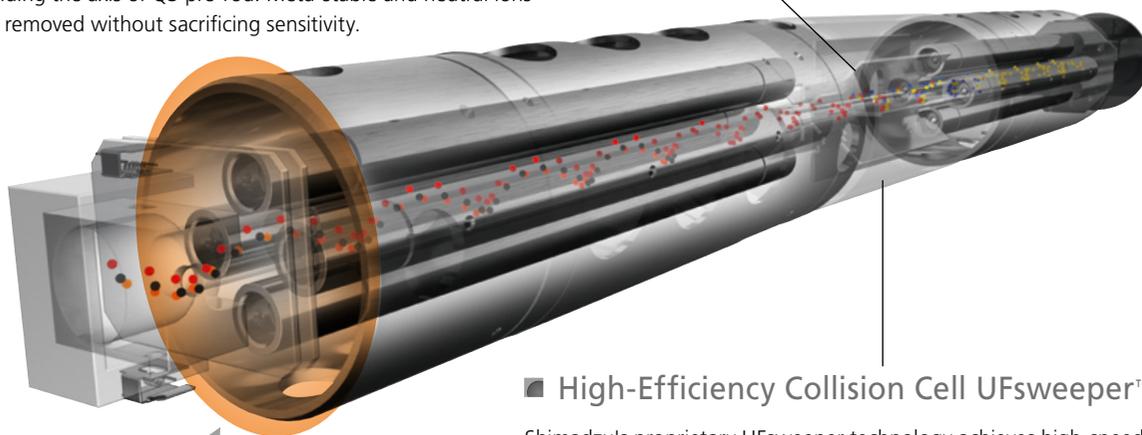
Repeatability with Polycyclic  
Aromatic Hydrocarbons (PAHs)



# Technology That Makes Possible the Simultaneous Analysis of Several Hundred Components

## ■ OFF-AXIS Ion Optics

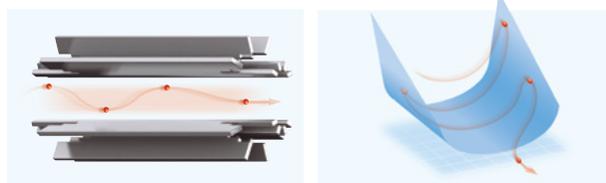
Lower detection limits are achieved by collision cell and OFF-AXIS Ion Optics, a patent technology, which is capable of bending the axis of Q3 pre-rod. Meta-stable and neutral ions are removed without sacrificing sensitivity.



Pre-rods prevent quadrupole contamination even with samples containing many matrices.

## ■ High-Efficiency Collision Cell UFsweeper™

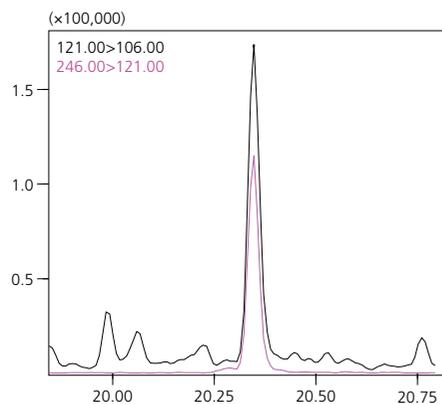
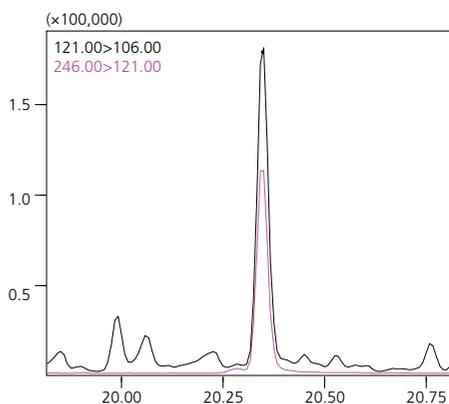
Shimadzu's proprietary UFsweeper technology achieves high-speed MRM analysis at speeds up to 800 transitions per second. It sweeps residual ions from the collision cell to provide high-efficiency CID and fast ion transport. Rapid ion removal minimizes cross-talk and enables trace analysis.



UFsweeper

## ■ Automatic Method Creation Smart MRM

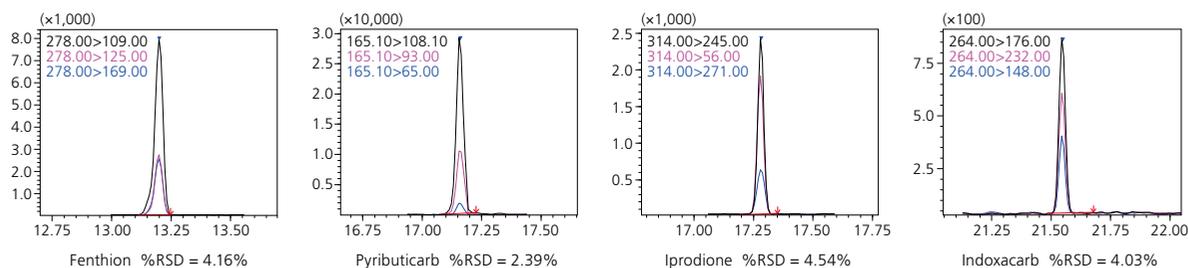
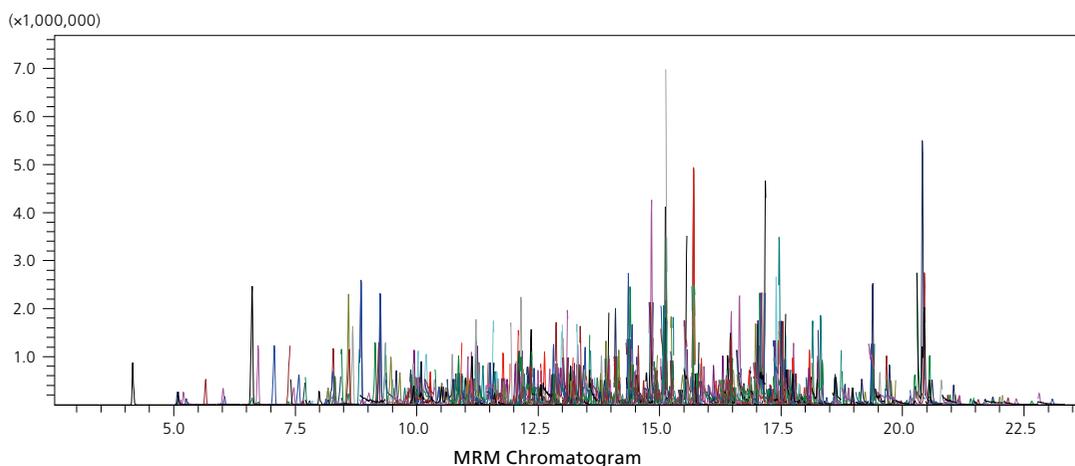
Smart MRM™ is a function that sets the optimal measurement time for each component, and automatically creates a method. Since only the data during the elution times of the targeted components is acquired, even when simultaneously analyzing several hundred components, detection occurs without any loss in sensitivity, even with trace concentrations.



Method for the Simultaneous Analysis of 20 Components      Method for the Simultaneous Analysis of 400 Components  
Dwell Time: 32 msec      Dwell Time: 2.7 msec

Analysis of Pharmaceutical in Blood Plasma (Nefiracetam)

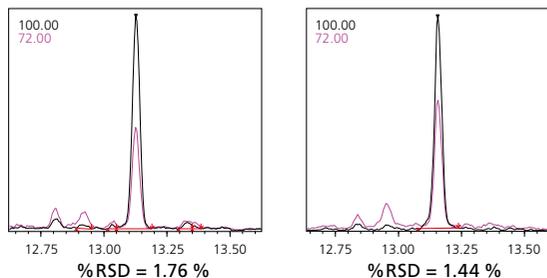
## Simultaneous Analysis of 439 Pesticides



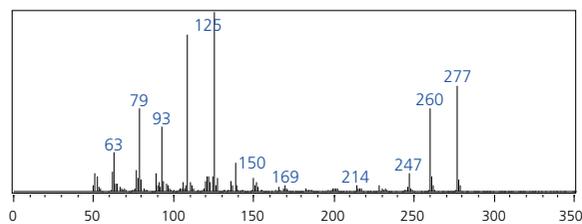
Mass Chromatogram and %RSD of Each Pesticide (5 pg/μL)

## High-Sensitivity Analysis by Single GC-MS Mode

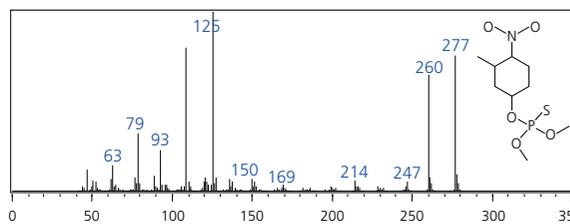
Due to a highly sensitive ion source and highly sensitive detector with overdrive lenses, the GCMS-TQ8040 NX is able to select and detect generated ions efficiently. That achieves high sensitivity not only for MRM measurements in the GC-MS/MS mode, but also for scan and SIM measurements in the GC/MS mode. In addition, pre-rods help prevent quadrupole contamination, so that stable sensitivity and mass spectra can be obtained even when samples containing many matrices are analyzed.



5 pg/mL Thiobencarb  
Left: GCMS-QP2020 NX, Right: GCMS-TQ8040 NX  
Reproducibility for n = 5



Scan Analysis Results for Fenitrothion



Mass Spectrum from NIST Library

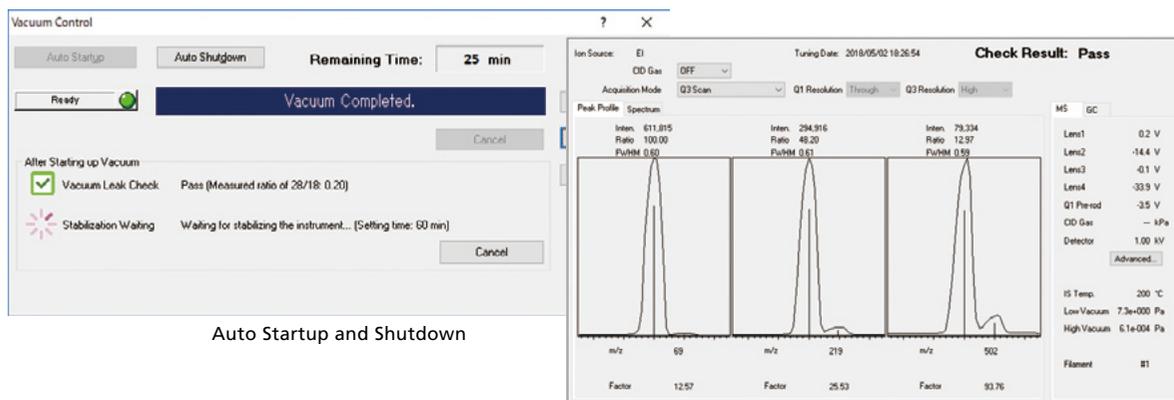
# Smart Productivity

The GC/MS is now a standard system for analysts, and a system can be used for a wide variety of applications. The active time management feature appropriately manages times when the system requires maintenance, or when system changes are being made, or the waiting time for a user when multiple users are waiting to use the system. This ensures more efficient use of the system and greater uptime.

## ■ Active-Time Management™ That Accurately Determines Operation Time

### Time Management during Instrument Startup/Shutdown

The mass spectrometer has to be operated in a vacuum condition, the startup and stopping of the system takes time depending on the condition. Determining this can be a challenge. Since the amount of time that the system takes when starting up or stopping is displayed in real time, it is easy to accurately determine when maintenance of the ion source or analysis is possible. Moreover, tasks that until now needed to be performed by the user, such as leak checks upon system startup and auto tuning, are now performed automatically.



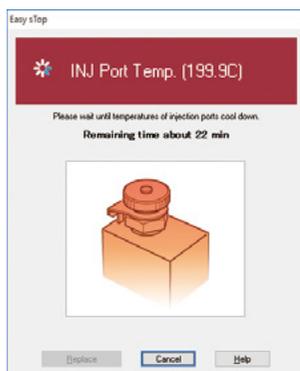
Auto Startup and Shutdown

Auto Tuning Check Result

### Time Management during Injection Port Maintenance

The Easy sTop function, used to safely maintain the sample injection port without releasing the vacuum, displays the remaining time (cooling-down time) when the septum or the insert can be replaced in real time. Maintenance time can be minimized by understanding the accurate remaining time.

Furthermore, by using a ClickTek nut on the top of the sample injection port, the port can be opened or closed without tools, by simply using fingers to twist a lever. That enables faster and easier insert replacement than ever before.



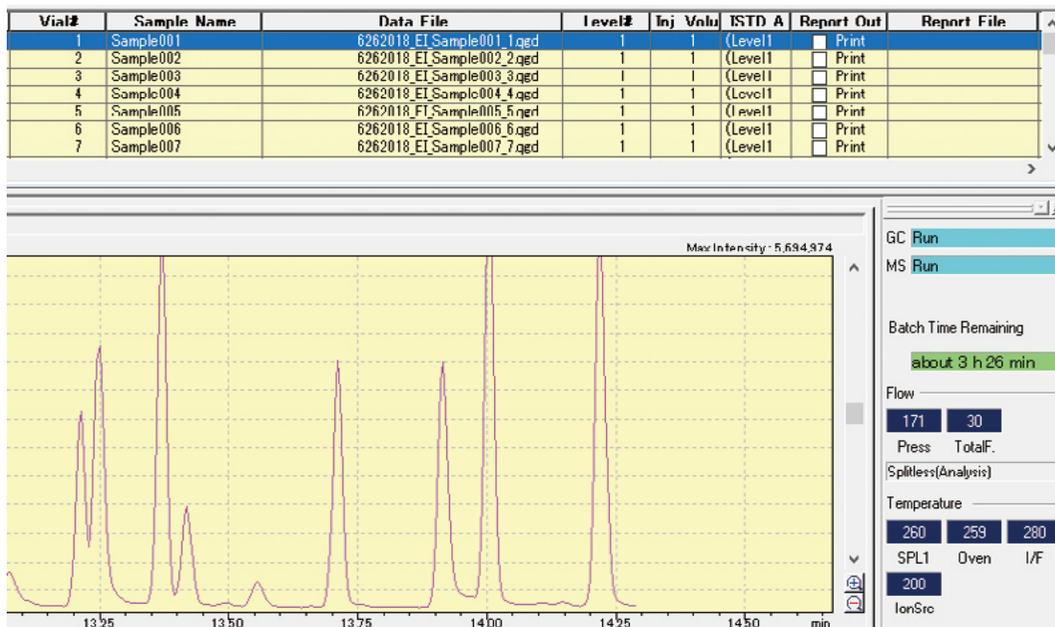
Easy sTop Function



ClickTek Nut

## Time Management for Continuous Analysis

By displaying the time required for continuous analysis in real time, the time when the current continuous analysis will finish can be accurately confirmed. This increases the instrument operating time (active time) by reducing standby time required during continuous analysis or while switching between different users. In addition, because this function makes it easier to schedule the timing for analysis preparations, such as sample preparation and pretreatment, based on the finish time of the previous analysis, it enables analytical processes to be performed more efficiently, which can help improve work-life balance.

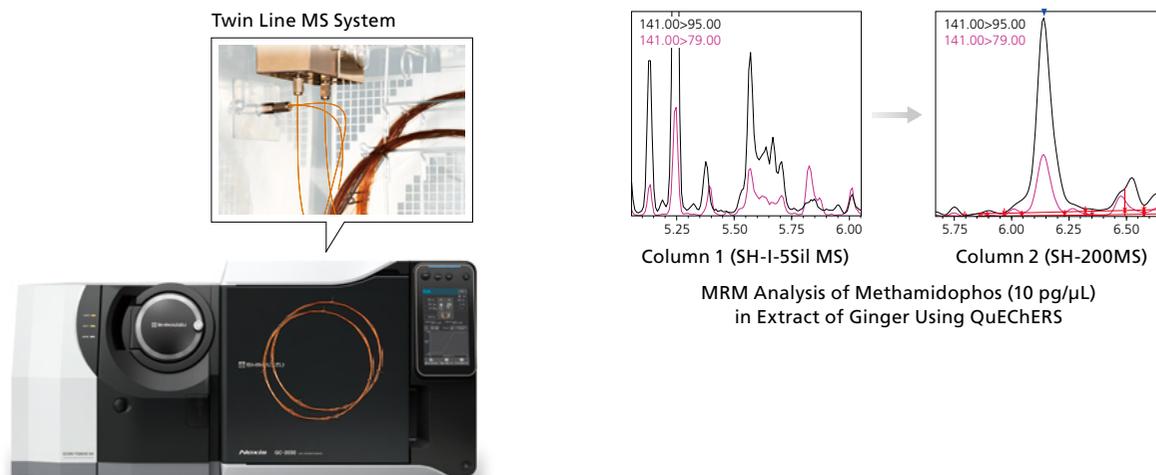


Time display for continuous analysis can be used only in liquid injection using AOC-20i.

## Simple Column Replacement Using the Twin Line MS System

By connecting the outlet ends of two different columns to the MS at the same, different application data can be acquired without shutting OFF the MS vacuum.

CID gas control is a method parameter, allowing acquisition of GC-MS and GC-MS/MS data in the same batch.



# Smart Operation

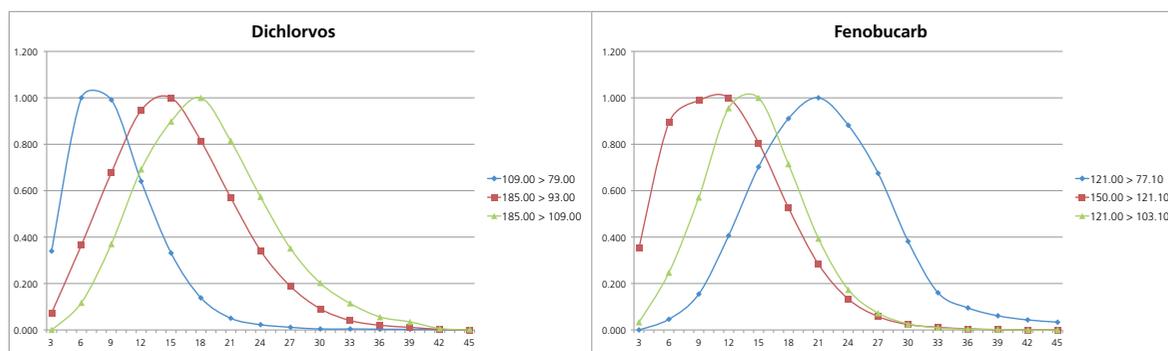
Creating an MRM analysis method requires determining the optimum transitions, collision energies, and other complicated parameters. Smart MRM, the method creation function, creates optimized analytical methods by using the transitions data in the "Smart Database" file. When you want to perform MRM measurements of components not contained in the database, the optimal transitions can be automatically searched for using the MRM Optimization Tool.

## MRM Optimization Tool

### ■ Optimize MRM Transitions Automatically

Determining and optimizing MRM transitions for new compounds can require significant development time. The "MRM Optimization Tool" automates the process by collecting product ion scan data and finding the optimum collision energy for each transition.

Once established, the transitions are registered to one of the Shimadzu "Smart Database" files, and the MRM or Scan/MRM methods are created using **Smart MRM**.



## Smart Database™

### ■ Method Management Achieved by Database File

The Shimadzu "Smart Database" is a database file for creating the method files using "Smart MRM" function. In addition to compound information and transitions, retention index can be registered in the database file. Method creation can be proceeded without calculating the retention time by analyzing the standard samples when using the Automatic Adjustment Retention Time (AART) function. In addition to MRM information, Scan and SIM ion information, mass spectra and calibration curve information from the internal standard method can also be registered in the database file. This allows users to create their own database easily.

Serial#	Type	Acq. Mode	ISTD Group	Level1 Conc (IS)	Method No.	Compound Name (E)	Ret. Index 1	Cas#	Ion1			
									Type	m/z	CE	Rat1
1	Target	MRM			1	Aldicarb deg.	881	0 - 00 - 0	T	115.1>68.0	8	100.00
2	Target	MRM			1	DCIP	1058	108 - 60 - 1	T	121.1>45.0	4	100.00
3	Target	MRM			1	Aldoxycarb deg.	1135	0 - 00 - 0	T	80.0>65.0	6	100.00
4	Target	MRM			1	Chlolfentazine deg.	1182	0 - 00 - 0	T	137.0>102.0	14	100.00
5	Target	MRM			1	Hymexazol	1196	10004 - 44 - 1	T	99.0>71.0	8	100.00
6	Target	MRM			1	Methamidophos	1236	10265 - 92 - 6	T	141.0>95.0	8	100.00
7	Target	MRM			1	Dichlorvos	1253	62 - 73 - 7	T	109.0>79.0	8	100.00
8	Target	MRM			1	Nereistoxin	1283	0 - 00 - 0	T	149.1>71.1	8	100.00
9	Target	MRM			1	Allidochlor	1296	93 - 71 - 0	T	132.1>56.0	8	100.00
10	Target	MRM			1	Dichtobenil	1358	1194 - 65 - 6	T	170.9>136.0	14	100.00
11	Target	MRM			1	EPTC	1364	759 - 94 - 4	T	189.1>128.1	4	100.00
12	Target	MRM			1	Biphenyl	1394	92 - 52 - 4	T	154.1>128.1	22	100.00
13	Target	MRM			1	Propamocarb	1398	24579 - 73 - 5	T	188.2>72.0	4	100.00

# Smart MRM

## Automatic Method Creation



The Smart MRM technology automatically creates methods with measurement times optimized for each component based on the Smart database. The Automatic Adjustment of Retention Time (AART) function incorporated in the system estimates retention times with high accuracy. When creating methods for simultaneous multicomponent analysis, the complicated process of configuring measurement parameters made it difficult to prepare appropriate methods. By using the Smart MRM function, however, it is possible to automatically create methods in which data are acquired with high sensitivity only during the elution time of the target components. In addition to MRM methods, SIM methods can be created.

**MS Table Parameter**

**MRM, SIM Parameter**

Loop Time (MRM, SIM): 0.30 sec

Required Processing Time: R.T.s: 0.30 min

Scan Mode:  ON  OFF

**Scan Parameter**

Event Time of Scan: 0.10 sec

Scan Range: Start m/z: 46, End m/z: 900

Acquisition Time: Start R.T.: 2, End R.T.: 28 min

**MRM Transition Table:**

Serial	Type	Acq. Mode	STD Group	Level Class (ms)	Method No.	Compound Name (E)	Ret. Index 1	Ret. Index 2	Ret. Index 3	Ret. Time	Case	Type	m/z	CE	...
1	Target	MRM		1	1	Adicarb-dep.	881				0-00-0	T	115-186.0	8	5
2	Target	MRM		1	2	PCP	1009	1070	1080		00-00-1	T	121-145.0	4	5
3	Target	MRM		1	3	Alloycarb-dep.	1135	1142	1141		0-00-0	T	60-049.0	5	5
4	Target	MRM		1	4	Chlofexolol-dep.	1182	1189	1183		0-00-0	T	107-0-100.0	14	5
5	Target	MRM		1	5	Hexamazol	1198	1202	1199		0004-44-1	T	80-571.2	5	5
6	Target	MRM		1	6	Methemphos	1258	1258	1254		0006-50-8	T	141-0-95.0	3	5
7	Target	MRM		1	7	Dichlorvos	1259	1256	1254		62-F3-7	T	109-0-79.0	8	5
8	Target	MRM		1	8	Hexetholol	1283	1287	1275		0-00-0	T	149-1-71.1	8	5
9	Target	MRM		1	9	Amoxiclor	1286	1300	1294		60-71-9	T	132-0-60.0	8	5
10	Target	MRM		1	10	Dioxocool	1360	1361	1360		1184-65-8	T	170-3-150.0	14	5

Parameter Setting

## Automatic Adjustment of Compound Retention Time (AART)

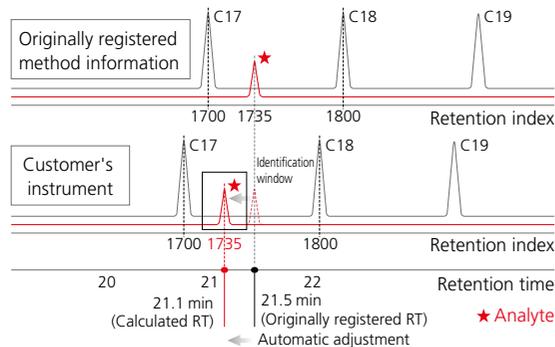
(Automatic Adjustment of Retention Time)

**Compound Name (E) Ret. Time**

200	Pirimiphos ethyl (3.3 ms)
201	Isopropalin (3.3 ms)
202	Isodrin (3.3 ms)
203	Cyprodinil (3.3 ms)
204	Isolfenphos-methyl (3.5 ms)
205	MGK 264-2 (3.3 ms)
206	(E)-Chlorfenvinphos (3.3 ms)
207	Dimethametryn (2.7 ms)
208	Metazachlor (2.7 ms)
209	Pendimethalin (2.7 ms)
210	Ethiozazole (2.8 ms)
211	Antiazole (2.8 ms)
212	Penconazole (2.7 ms)
213	Heptachlor-endo-epoxide (2.7 ms)
214	oxy-Chlordane (2.7 ms)
215	Chlortalolol (2.7 ms)
216	(Z)-Pyrifenoxy (2.7 ms)
217	Thiabendazole (2.7 ms)
218	Allethrin-1,2 (2.7 ms)
219	Phosfolan (2.5 ms)
220	Tolyfluandis (2.7 ms)
221	Heptachlor-endo-epoxide (2.7 ms)
222	Bromfeninfos-methyl (2.7 ms)

Automatic Estimation of Retention Times

Dwell Time Optimization



The AART function adjusts the retention times of target components based on linear retention indices (LRI) and the retention times of n-alkanes. The AART function easily adjusts acquisition and processing method parameters simultaneously.

Automatic Creation of Analysis Methods

Compound Name	Acq. Mode	Event Time(sec)	Ch1 m/z	Ch1 CE	Ch2 m/z	Ch2 CE	Ch3 m/z	Ch3 CE	
44-14	MGK 264-2	MRM	0.018	164.10>98.00	12.00	111.10>82.00	8.00	164.10>87.00	8.00
44-15	(E)-Chlorfenvinphos	MRM	0.018	323.00>267.00	16.00	267.00>159.00	18.00	267.00>203.00	12.00
44-16	Dimethametryn	MRM	0.018	212.10>122.10	12.00	212.10>94.00	22.00	212.10>71.00	18.00
44-17	Metazachlor	MRM	0.018	209.10>132.10	18.00	133.10>117.10	24.00	211.10>132.10	20.00
45-1	Diphenamid	MRM	0.014	167.10>152.10	20.00	238.10>167.10	8.00	238.10>72.00	16.00
45-2	Fosthiazate-2	MRM	0.014	195.00>103.00	10.00	195.00>60.00	22.00	195.00>139.00	6.00
45-3	Pirimiphos ethyl	MRM	0.014	304.10>168.10	12.00	318.10>166.10	12.00	318.10>182.10	12.00
45-4	Isopropalin	MRM	0.014	280.10>238.10	8.00	280.10>183.10	18.00	280.10>166.10	16.00
45-5	Isodrin	MRM	0.014	192.90>157.00	20.00	192.90>123.00	26.00	262.90>192.90	28.00
45-6	Cyprodinil	MRM	0.014	224.10>208.10	16.00	224.10>197.10	22.00	224.10>181.10	14.00
45-7	Isolfenphos-methyl	MRM	0.010	199.00>121.00	14.00	241.10>121.10	22.00	0.00>0.00	0.00
45-8	MGK 264-2	MRM	0.014	164.10>98.00	12.00	111.10>82.00	8.00	164.10>87.00	8.00
45-9	(E)-Chlorfenvinphos	MRM	0.014	323.00>267.00	16.00	267.00>159.00	18.00	267.00>203.00	12.00
45-10	Dimethametryn	MRM	0.014	212.10>122.10	12.00	212.10>94.00	22.00	212.10>71.00	18.00

# Multianalyte Data Analysis with More Efficiency Using LabSolutions Insight™

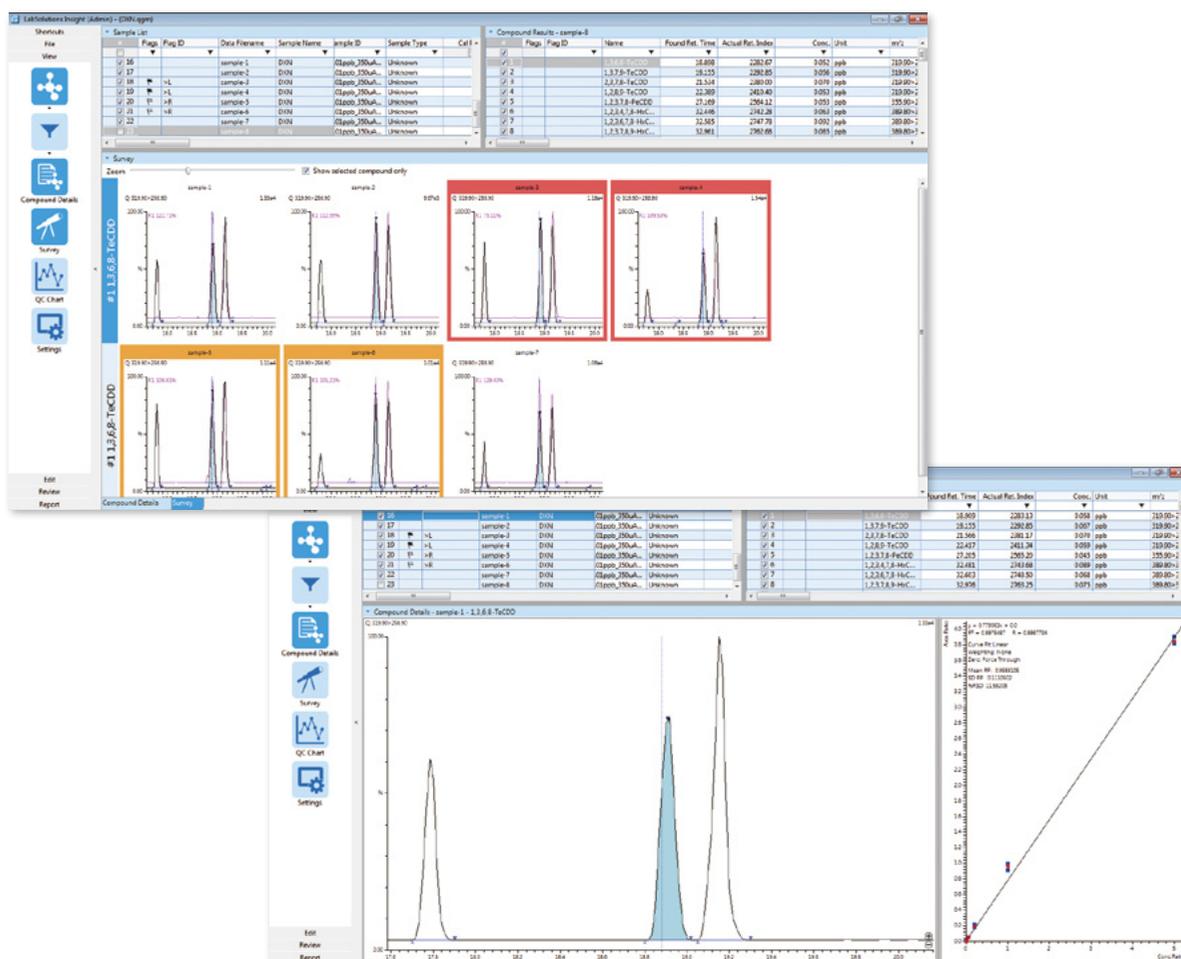
LabSolutions Insight quantitative analysis support software includes functionality for enhancing the throughput of multianalyte data analysis, making it especially helpful for routine analysis. Quantitative results for a series of data sets can be displayed at the same time for data analysis. Chromatograms for each set of sample data can be displayed side-by-side for each compound, making it easy to confirm peak detection and quantitative results. Color-coded flagging functionality makes it easy to quickly see peaks from any of multiple analytes that exceed criteria values. That drastically decreases the number of peaks that need to be checked and improves the efficiency of quantitative analysis processes.

## ■ More Efficient Multianalyte Data Analysis

Users can select the optimal method for displaying data based on their workflow. For example, data analysis windows can be displayed for each target compound or each set of measurement data, or quantitation or area values can be displayed as a list. If necessary, quantitative analysis can be repeated with peaks directly corrected, which provides intuitive operability.

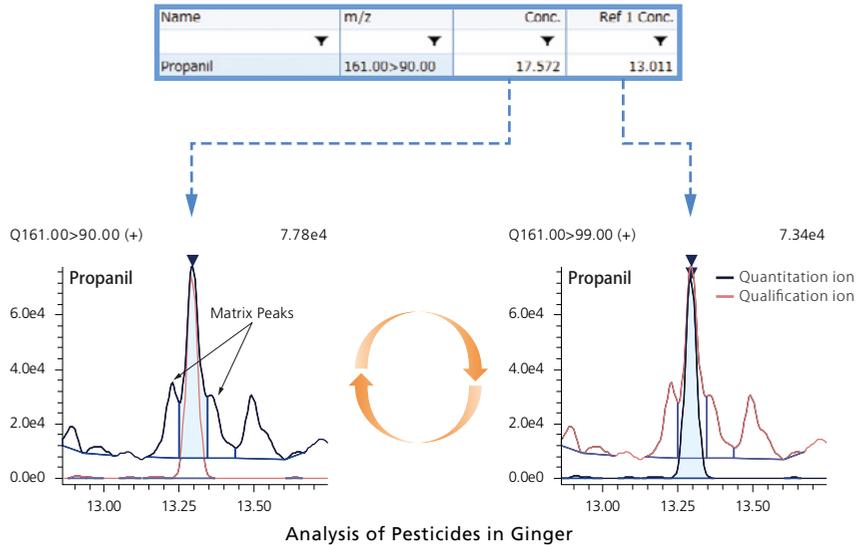
## ■ Visualization of Quantitative and Accuracy Control Results

Quantitative and accuracy control results can be presented more clearly by using the flagging function to color-code result values that exceed specified criteria values or by only displaying flagged results. Five levels of criteria values can be indicated for quantitative results, making it easy to confirm the corresponding criteria value range for the detected compounds. Flagging immediately reflects results from any corrections made to manual peak integration or calibration curves.



## ■ Easy Control of Quantitation and Reference Ions

Analysts can update retention times and reference ion ratios quickly and easily from a single standard or a group of standards. It is also easy to reassign quantitation ions as needed for method development purposes or because of unexpected matrix interferences.



## ■ Status Review Function

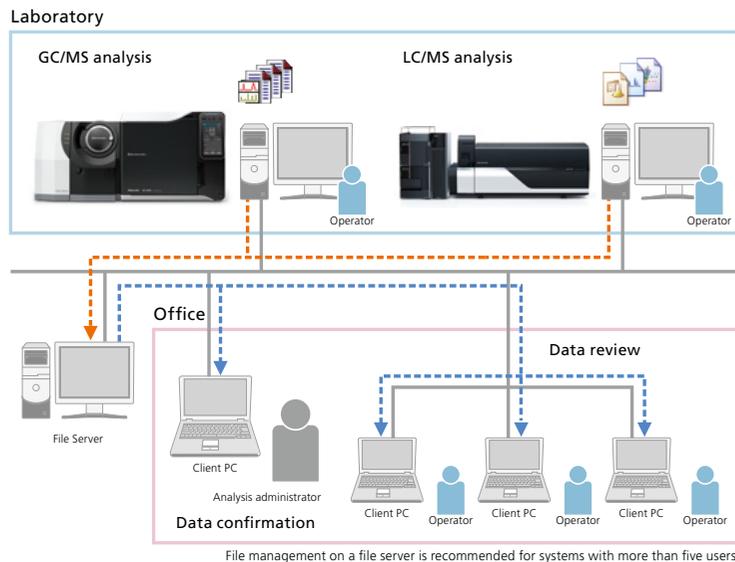
This function can be used to specify the status of all compounds and samples for their management. By specifying a status, the progress of data analysis work can be accurately recorded and reported.

#	Flags	Data Filename	Status	Sample Type
<input checked="" type="checkbox"/>		Conc-3_001	Pending	Standard
<input checked="" type="checkbox"/>		Conc-3_002	Accept	Standard
<input checked="" type="checkbox"/>		Conc-3_003	Review	Standard
<input checked="" type="checkbox"/>		Unknown-1	Rerun	Unknown

#	Name	Status
<input checked="" type="checkbox"/>	MPA-gluc	Pending
<input checked="" type="checkbox"/>	d3-MPA-	Pending
<input checked="" type="checkbox"/>	MPA	Pending
<input checked="" type="checkbox"/>	d3-MPA	Pending

## ■ Network Support

Data acquired from multiple systems can be reviewed or confirmed using client computers connected via a LAN or other network. If multiple systems are used, data obtained from each system can be reviewed from any client computer. Even in the case of multiple analysts using the same system, the ability to separate analytical work from measurement work improves efficiency.



## Smart Database Series Enables Accurate Analysis Using MRM

GC-MS/MS database series specialized for various fields supports your analysis with ease and accuracy. These databases contain pre-optimized MRM transitions and collision energies required for GC-MS/MS analysis, allowing users to start an analysis immediately just by using the AART function to automatically modify the retention times.

### ● Smart Pesticides Database™

It covers the pesticides (530 compounds) subject to GC-MS analysis and used inside and outside Japan. The database also contains information on compounds that can be used as internal standards. Therefore, it also supports analysis with the internal standard method.



### ● Smart Metabolites Database™

The database contains 627 compounds including metabolites contained in food, blood, urine and cells. It also contains information on the stable isotopes of 38 major metabolites, which can be used as internal standards.



### ● Smart Aroma Database™

511 compounds that contribute to aroma are registered in the database. This database supports various aroma analysis, such as detecting aroma compounds from scan measurements and high-sensitivity target analysis using MRM and SIM.



### ● Smart Forensic Database™

The database is registered with 486 forensic toxicological substances often involved in poisonings, such as drugs of abuse, psychotropic drugs, pharmaceuticals, and pesticides.



### ● Smart Environmental Database™

The database contains information on 527 compounds including polychlorinated biphenyl, brominated flame retardants, dioxins, polycyclic aromatic hydrocarbons, and organochlorine pesticides, as well as their stable isotope labeled compounds.



## Quick-DB™ Series Enables Quick Screening Without Using Standards

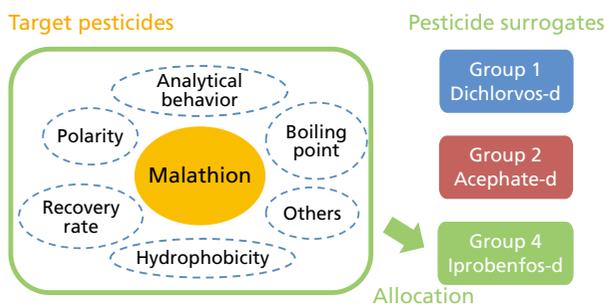
Preregistered with calibration curve information from the internal standard methods, this database allows users to calculate quantitative values without analyzing standard samples. It can be used for screening when quick confirmation of quantitative results is required.

### ● Quick-DB GC/MS Residual Pesticides Database

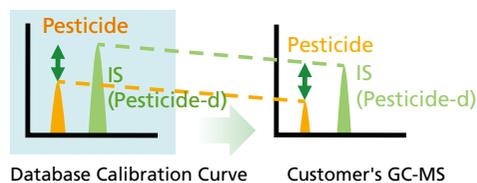
The database contains information on calibration curves created using pesticide surrogates as the internal standards, thus enabling the simultaneous screening of 491 residual pesticides without using standard samples. The registered calibration curves have been created by grouping target pesticides based on similar behavioral and physical properties, and allocating pesticide surrogates with similar physical properties to each group as internal standard substances. This allows highly accurate quantitative values to be calculated.



Allocation of Pesticide Surrogates  
Based on Physical Properties of Target Pesticides



Sensitivity Variation Adjustments Using Pesticide Surrogates



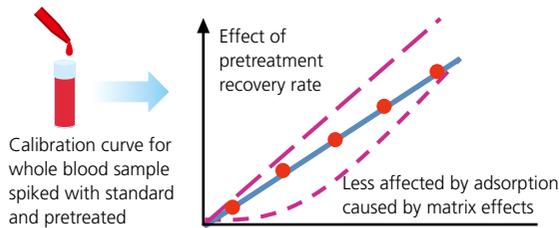
Pesticide surrogates can also be used to adjust differences in target pesticide responses observed in calibration curves and a customer's instrument due to variations in GC-MS/MS sensitivity.

## ● Quick-DB Forensic Toxicology Database

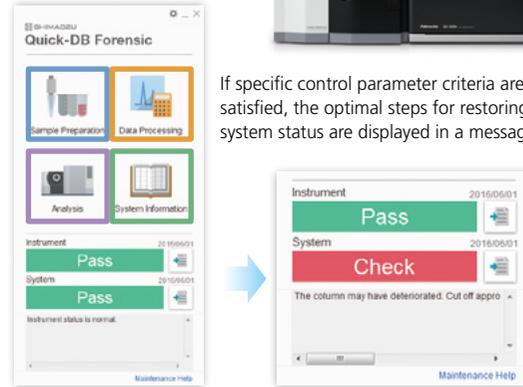
This database contains information on sample preparation, data acquisition, and analysis of 68 compounds often involved in poisonings. Due to the simple QuEChERS method used for the sample preparation, even first-time users can pretreat samples easily. The performance control function, which automatically assesses the system status, quickly determines problematic areas. As a result, users can analyze toxicological substances while consistently maintaining the highest status level.

### Using a Calibration Curve for a Pretreated Sample to Correct for Recovery Rates

By using the calibration curve information from a pretreated sample, accurate quantitative values can be obtained. The calibration curve information is used to correct differences in recovery rates for each target compound or correct for effects caused by adsorption, which occurs when creating calibration curves using standards.



If specific control parameter criteria are not satisfied, the optimal steps for restoring the system status are displayed in a message box.



Quick-DB Forensic Launcher Screen

## ● Off-Flavor Analyzer

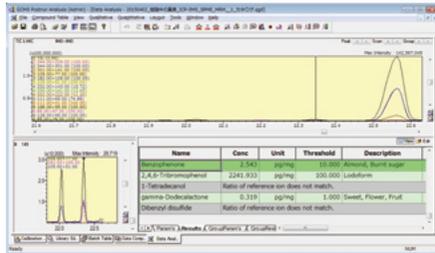
This analysis system contains information on the major odor-causing substances identified from previous problems and associated sensory information, thus enabling the reliable identification of odor-causing substances. It allows users to calculate quantitative values easily without using standard samples, and to identify odor-causing substances through comparison with registered odor thresholds. The system also supports the use of a sniffer, enabling the efficient confirmation of odors using the predicted retention time display function.

In addition, support is provided for a total system, including pretreatment units such as HS, SPME, and thermal desorption units using MonoTrap™.

Compound Name (E)	Ret. Index 1	Comment (E)	Threshold
Benzophenone	2472	Almond, Burnt sugar	10
2,4,6-Tribromophenol	2000	Lodoform	100
L-Tetraolactone	2188	Coconut	1000
gamma-Dodecalactone	2384	Sweet, Flower, Fruit	1
Chenopodiolide	3022	Flour	1

Primary odor components      GC/MS analytical conditions      Sensory information

### Comparison of Concentration to Odor Threshold Values



Odor-causing substances can be identified through comparisons of odor thresholds with the concentrations of off-flavor components identified in a chromatogram.

Name	Conc	Unit	Threshold	Description
Benzophenone	2.543	pg/mg	10.000	Almond, Burnt sugar
2,4,6-Tribromophenol	2241.933	pg/mg	100.000	Lodoform

#### Under Threshold Value

##### Benzophenone

Concentration/Threshold=Odor threshold value  
2.543/10.000=0.254

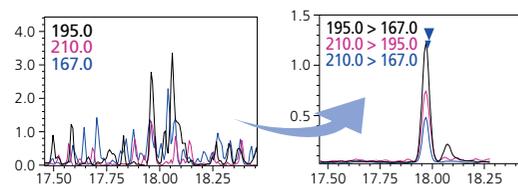
#### Over Threshold Value

##### 2,4,6-Tribromophenol

Concentration/Threshold=Odor threshold value  
2241.933/100.000=22.419



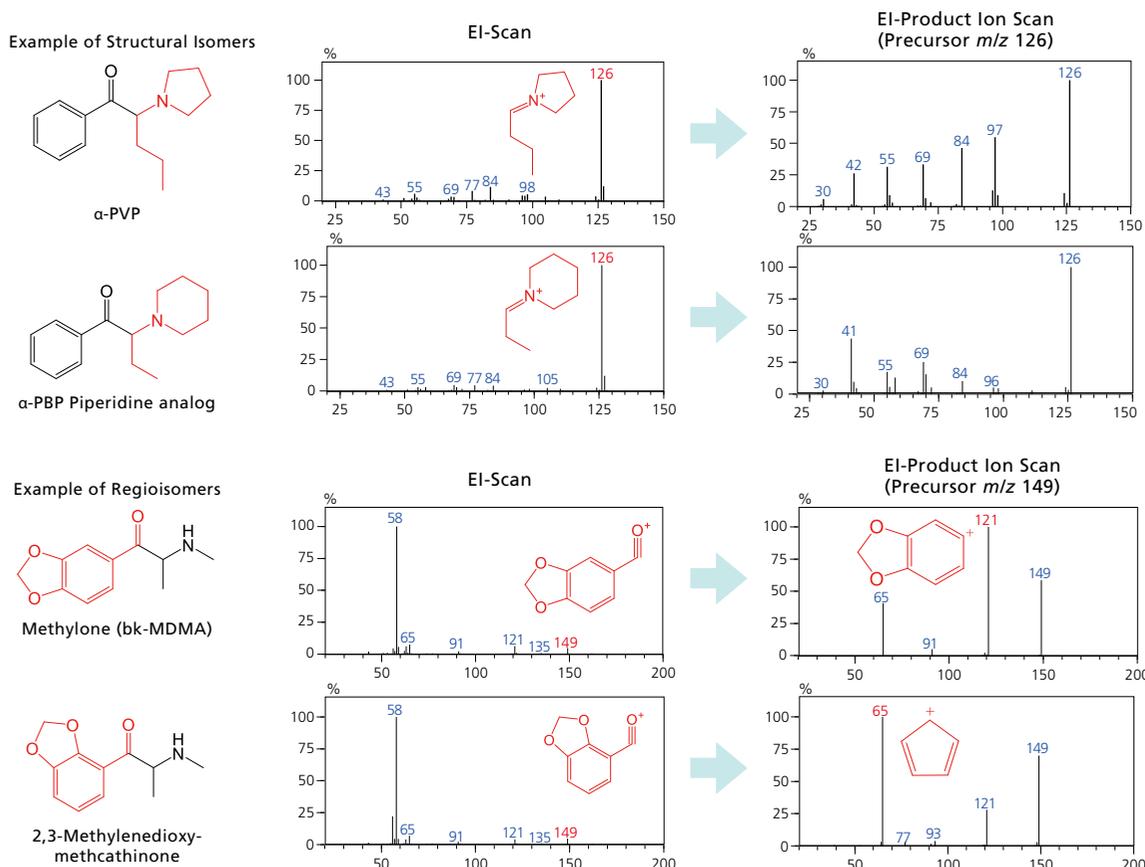
Since some odor components have a low odor threshold, low concentration levels need to be detected to identify the causative substances. High-sensitivity MRM/SIM analysis by GC-MS(/MS) can reliably detect even trace components near the odor threshold (a few pg/g).



Mass Chromatograms of 2,4,6-Trichloroanisole (estimated concentration of 18.166 pg/g) in Food with an Odd Odor (Left: Scan analysis, Right: MRM analysis)

# Qualitative Analysis Using GC-MS/MS

GC-MS/MS allows users to freely select ions cleaved by electron ionization (EI), and then cleave precursor ions via collision induced dissociation (CID), thus enabling the detailed analysis of partial structures. A product ion scan can be used to easily discriminate structural isomers and regioisomers, which are hard to identify with an EI mass spectrum obtained via GC/MS. This mode is optimal for predicting partial structures.

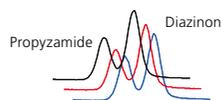


## High-Speed Scan Control Technology

### Advanced Scanning Speed Protocol (ASSP™)



Newly Patented Technology (ASSP)



Black: 1,111 u/sec  
Red: 5,000 u/sec  
Blue: 10,000 u/sec

Equipped with a function to automatically optimize the rod bias voltage during high-speed data acquisition, the system can collect data stably through scans as well as product ion scans at 20,000 u/sec (patent: US6610979).

With the GCMS-TQ8040 NX, ten or more product ion scans can be configured for a single measurement, and three or more user-specified analysis modes (Scan, MRM, product ion scan) can be combined.

	Compound Name	Start Time (min)	End Time (min)	Acq. Mode	Event Time(sec)	Scan Speed	Start m/z	End m/z	Precursor m/z	CE
1-1		2.30	43.00	Q3 Scan	0.050	10000	43.00	500.00		
1-2		2.30	43.00	MRM	0.050					
1-3	Amine m/z44	2.30	43.00	Product Ion Scan	0.005	20000	29.00	45.00	44.00	15.00
1-4	Amine m/z58	2.30	43.00	Product Ion Scan	0.005	20000	29.00	59.00	58.00	15.00
1-5	Amine m/z72	2.30	43.00	Product Ion Scan	0.008	20000	29.00	73.00	72.00	15.00
1-6	Amine m/z86	2.30	43.00	Product Ion Scan	0.008	20000	29.00	87.00	86.00	15.00
1-7	Amine m/z98	2.30	43.00	Product Ion Scan	0.010	20000	29.00	99.00	98.00	15.00
1-8	Amine m/z100	2.30	43.00	Product Ion Scan	0.010	20000	29.00	101.00	100.00	15.00
1-9	Amine m/z112	2.30	43.00	Product Ion Scan	0.010	20000	29.00	113.00	112.00	15.00
1-10	Amine m/z114	2.30	43.00	Product Ion Scan	0.010	20000	29.00	115.00	114.00	15.00
1-11	Amine m/z126	2.30	43.00	Product Ion Scan	0.010	20000	29.00	127.00	126.00	15.00
1-12	Amine m/z128	2.30	43.00	Product Ion Scan	0.010	20000	29.00	129.00	128.00	15.00
1-13	Amine m/z140	2.30	43.00	Product Ion Scan	0.010	20000	29.00	141.00	140.00	15.00
1-14	Amine m/z142	2.30	43.00	Product Ion Scan	0.015	20000	29.00	143.00	142.00	15.00

UFMS  
ULTRA FAST MASS SPECTROMETRY

# Enhanced Support System for Data Management

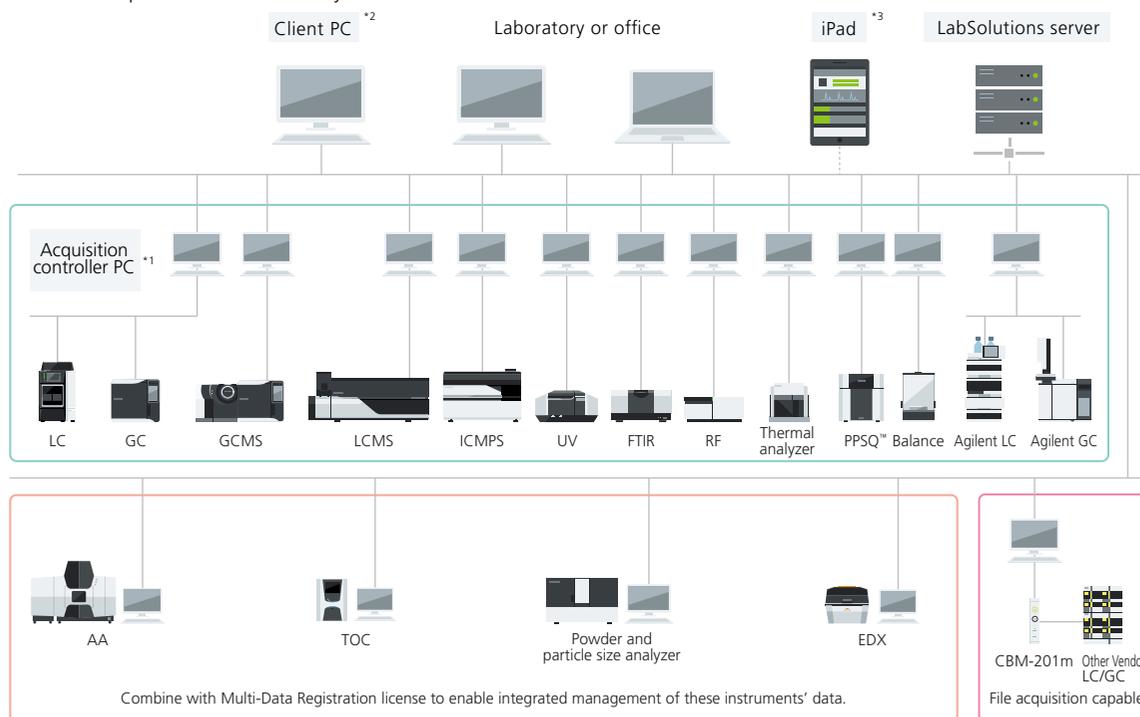
LabSolutions™ DB/CS Realizes Complete Data Integrity\*

LabSolutions DB/CS is the integration software for analytical instruments that complies with regulations regarding electronic records and signatures, such as "FDA 21 CFR Part 11" and "ER/ES guidelines".

Data management with LabSolutions prevents overwriting or deleting analysis data. It also offers a complete suite of advanced security features to provide an optimal solution for data integrity.

## Network System: LabSolutions CS

Data acquired from multiple systems can be reviewed or confirmed using client computers connected via a LAN or other network. If multiple systems are used, data obtained from each system can be reviewed from any client computer. Even in the case of multiple analysts using the same system, the ability to separate analytical work from measurement work improves work efficiency.



\*1 The acquisition control PC controls analytical instruments. It can also be used to send analytical instructions and perform post-run analysis, just like a client PC.

\*2 If a terminal service is used, then LabSolutions software does not need to be installed on client PCs.

\*3 If an iPad is used, then XenApp from Citrix must be installed.

## Standalone Database System: LabSolutions DB

LabSolutions DB manages data by connecting a computer with analysis instruments, which do not have network connections. It is recommended for facilities that do not require network connections and want to be ER/ES compliant with one computer.

\*LabSolutions DB/CS is optional software that provides enhanced data integrity support. Some analysis systems and functions are not supported in contrast to the standard workstation software GCMSSolution.

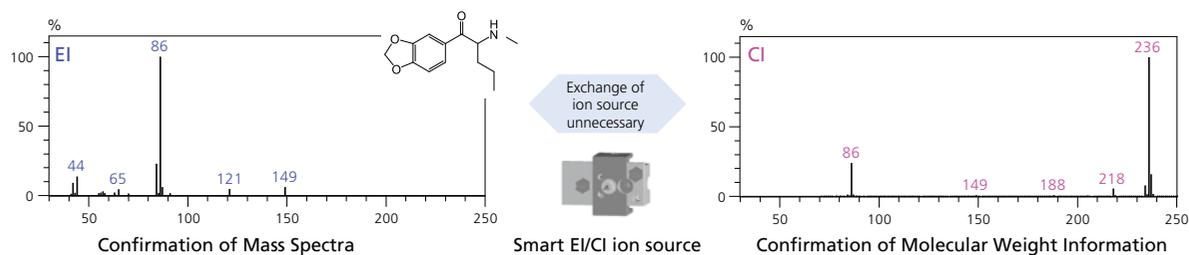
# Configure Optimal Analysis Systems to Meet Your Needs

For GC-MS/MS analysis, different system configurations may be required depending on the application and sample-introduction needs. The GCMS-TQ8040 NX offers a wide variety of system configurations and sample-introduction devices to enable an expanded range of applications.

## Smart EI/CI Ion Source Easily Switches Between EI and CI Methods

The Smart EI/CI ion source has been developed in order to acquire CI data without switching the ion source, and without losing the sensitivity of EI, which is most commonly used.

Even when it is difficult to perform identification with the EI mode using the mass spectral library, molecular weight information can be obtained from CI data, thus helping in the estimation of unknown compounds.



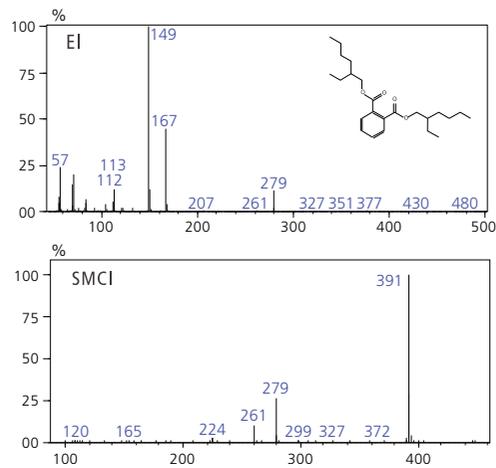
## SMCI Unit

SMCI (Solvent Mediated Chemical Ionization) is a soft ionization method for GCMS. The headspace reagent gas from the sample bottle is introduced into the GCMS ionization unit to be ionized, which then causes chemical ionization (CI) of the target molecule via protonation.\* Previous CI methods have required the use of flammable reagent gas cylinders, but SMCI can be carried out with a general organic solvent such as methanol or acetonitrile, together with nitrogen or argon gas. This results in greater safety and lower running costs.



SMCI unit + GCMS-TQ8040 NX

SMCI can obtain the same results as previously-existing CI methods, but is less dependent on the compound. For example, it has been difficult to verify the molecular weight of phthalate esters using EI or previously-existing CI method, whereas SMCI can identify the quasi-molecular ions.



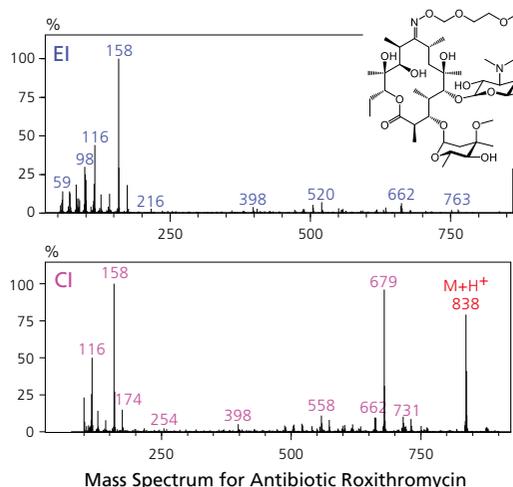
The mass spectrum of bis(2-ethylhexyl) phthalate (MW=390) obtained using different ionization methods

## DI-2010 Direct Inlet System

Direct sample injection (DI) is a method in which a sample is injected directly into the ion source without passing through the gas chromatograph (GC). This is an effective method for measuring the mass spectra of synthetic compounds, and can be used easily with a typical GC-MS configuration. By using this in combination with Smart EI/CI ion source, EI and CI mass spectra can easily be collected.



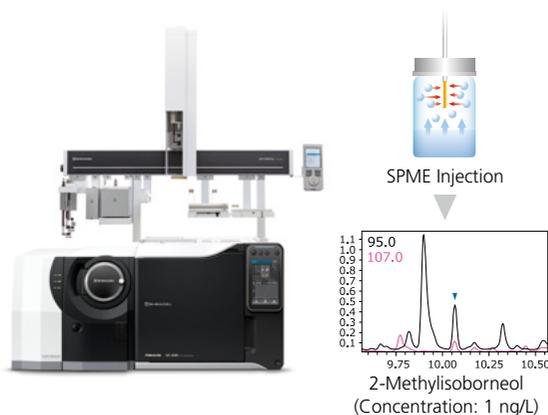
Components that are thermally degradable or difficult to vaporize are not suited to GC analysis. However, their mass spectra can be obtained easily using the DI probe.



## ■ AOC-6000 Plus Multifunctional Autosampler System

The AOC-6000 Plus supports three sample injection methods: liquid sample injection, headspace (HS) injection, and solid phase micro extraction (SPME) injection, so samples in a variety of forms can be analyzed. It allows the sample injection method to be switched automatically, enabling different sample injection methods to be combined in a continuous operation.

With the automatic syringe exchange and vial mixing function, standard samples can be prepared automatically with a variety of dilution levels, and everything from the creation of calibration curves to the quantitative determination of unknown samples can be fully automated.



## ■ HS-20 NX Headspace Analysis System

The HS-20 NX headspace sampler provides strong backup for the analysis of volatile components at every stage from research to quality control departments. The high-sensitivity electronic cooling trap enables quantitative and qualitative determination of trace components that cannot be detected with a conventional headspace sampler.

The HS-20 NX transfer line is built into the GC unit, which makes it easy to combine the HS-20 with the AOC-20 liquid sample injector, as well as to switch between these units.



## ■ OPTIC-4 Multimode Sample Inlet System

The OPTIC-4 multimode sample inlet is a GC injection port that enables a variety of sample injection modes for GC-MS, including large-quantity injection, inlet derivatization, thermal desorption, and DMI (difficult matrix introduction).

Combining this with an autosampler enables automatic replacement of inserts, improving productivity in multisample analyses.



## ■ TD-30 Thermal Desorption System

Thermal desorption systems heat samples in a sample tube and then concentrate the thermally desorbed gases before injection into a GC-MS. They are commonly used to measure volatile organic compounds (VOCs) in the atmosphere or measure trace components that are generated from plastic or other samples.

The TD-30R can accommodate 120 samples for excellent processing capacity and offers outstanding expandability, such as functionality for retrapping components or for automatically adding an internal standard substance.



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